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Field Effect Transistor in Nanoscale

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14. ABSTRACT
Weakly coupled molecular junctions are quite active and important field of research as they exhibit various non-linear transport phenomena. The principal investigator has investigated carrier transport through weakly coupled B2C2N2H6 (Benzene analogues) and BxCyNz (Napathalene analogues with x+y+z=10) molecules using quantum many body approach coupled with kinetic (master) equations. Interestingly, various types of non-linear current voltage characteristics, such as, negative differential conductance (NDC), rectifications, Coulomb staircase, which are hallmark of multistate transport devices, have been obtained. Source-drain voltage induced change in the occupation probabilities of low-lying many body states which are different in nature towards carrier transport, directly control the net current flowing through the molecular junctions. A few descriptors (the electrode contact points on two rings in case of naphthalene analogues) which directly dictate the behaviour of I-V characteristics were also found. These predictions would help the experimentalists to know what to expect depending on where the contacts are being probed.

Further investigation on the effect of different kinds of perturbations such as, gate voltage and perpendicular optical magnetic field, over carrier flow through the molecular bridges was done. Interestingly, the principal investigator found that depending on the strength of the applied optical magnetic field, several phenomena, such as, switching off current, suppression of NDC features appear in the devices. Fundamentally, the applied perturbations modify both the site charge densities as well as occupation probabilities of transport active channels, resulting in a quite significant alteration in transport behaviour of these molecular junctions.

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Theory, Nanoscale, Field Effect Transistor (FET), Devices, Density Functional Theory (DFT), Non-equilibrium Green Function

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Abstract: Short summary of most important research results that explain why the work was done, what was accomplished, and how it pushed scientific frontiers or advanced the field. This summary will be used for archival purposes and will be added to a searchable DoD database.

Weakly coupled molecular junctions are quite active and important field of research as they exhibit various non-linear transport phenomena. We have investigated the carrier transport through weakly coupled B2C2N2H6 (Benzene analogues) and $B_xC_yN_z$ (Napathalene analogues with x +y+z=10) molecules using quantum many body approach coupled with kinetic (master) equations. Interestingly, various types of non-linear current voltage characteristics, such as, negative differential conductance (NDC), rectifications, Coulomb staircase, which are hallmark of multistate transport devices, have been obtained. Source-drain voltage induced change in the occupation probabilities of low-lying many body states which are different in nature towards carrier transport, directly control the net current flowing through the molecular junctions. We also found a few descriptors (the electrode contact points on two rings in case of naphthalene analogues) which directly dictate the behaviour of I-V characteristics. These predictions would help the experimentalists to know what to expect depending on where the contacts are being probed.

We further investigate the effect of different kinds of perturbations such as, gate voltage and perpendicular optical magnetic field, over carrier flow through the molecular bridges. Interestingly, we find that depending on the strength of the applied optical magnetic field, several phenomena, such as, switching off current, suppression of NDC features appear in the devices. Fundamentally, the applied perturbations modify both the site charge densities as well as occupation probabilities of transport active channels, resulting in a quite significant alteration in transport behaviour of these molecular junctions.

Introduction: Include a summary of specific aims of the research and describe the importance and ultimate goal of the work.

Molecular electronics, the investigation about the electronic properties of circuits made of individual molecules, have gained a huge research attention in past few decades [1,2]. Appearance of efficient switching [3], negative differential conductance (NDC)[4], rectification [5], spin-transport [6], spin-filtration [7], thermoelectric effect [8] in various molecular junctions evidently shows the potential of these nano-devices to be used as alternative of conventional silicon-based semiconductor electronics. Among all these fascinating properties, particularly, rectification and NDC characteristics have been explored quite thoroughly from very beginning of this field. A number of molecules strongly attached to the bulk electrodes have shown the efficient rectification and/or NDC, mainly due to (a) molecular asymmetric nature (donor-acceptor molecules)[9] (b) different electrode-molecule coupling strengths (asymmetric anchoring groups or electrodes)[10] (c) different spatial potential profiles [11] etc. Although these phenomena majorly appear for covalently bonded molecule-electrode systems (i.e. coherent tunnelling regime), recent experimental and theoretical investigations demonstrated them for weakly coupled molecular junctions also (sequential tunnelling regime) [12,13]. Small molecules (such as benzene), double quantum dots (like GaAs-based QDs) which are coupled weakly to metallic electrodes have shown their prominent rectification and NDC properties, due to various factors, such as, internal charge transfer, intrinsic molecular asymmetries, interference effects, Pauli spin-blocking etc [14-17].

Recently, the modulations of electron transport through these molecular junctions by including different kinds of optical, magnetic and electronic perturbations have found huge applications, as these perturbations control and tailor the current-voltage characteristics. The magnetic field induced tuning of current may appear from several factors, such as, tuning of interfering electronic degenerate states, modulation of the sharp transmission resonances etc. The electronic perturbations include the modulation of charge carriers by varying potential through a third electrode, called Gate electrode.

Theoretical modelling of these weakly coupled devices show that coherent non-equilibrium Green's function (NEGF)[18,19] formalism coupled with self-consistent field (SCF) approach is not adequate to reproduce experimental findings even at a qualitative level. Unlike strongly coupled systems, in these devices charging energies of molecules/QDs are much higher than electrode coupling and play a major role [20,21]. Consequently, these devices remain in Coulomb blockade (CB) regime where integral charge transfer dominates the electron transport through the device. The mostly used formalism to describe the molecular transport in CB regime is the quantum master or rate equation approach [22,23]. This formalism efficiently describes electron transport through many-body eigenstates of molecular device systems. Since in this limit, charging energy is much higher than the molecule/dot electrode coupling, in the kinetic equation method, we do not explicitly consider the electrode's coupling with the molecule/dot device.

Using this approach, Hettler et. al. have demonstrated the large NDC behaviour in weakly coupled benzene based molecular junctions [24]. Here, under finite bias, the radiative relaxation of electrons populate a particular many-body state which blocks the transport of current, resulting in the NDC in the

device. Darau et al. revisited the same system with generalized master equation approach, where strong interference effect appears to be the reason for the observed NDC behaviour [25]. Apart from molecules, donor-acceptor QDs in weak coupling regime have also been investigated thoroughly for their various non-linear transport characteristics. Parida et. al. used similar kinetic equation approach to investigate transport characteristics in donor-acceptor double QD systems [26]. In this study, the authors find increased population in the dark triplet state with increase in bias voltage and consequent reduction in the current transport, exhibiting a prominent NDC feature. Muralidharan et al. demonstrated the criterion to find NDC in these double QDs in terms of transition rates for populating and depopulating energetically transport-active many-body states [22]. Song et. al. have shown the appearance of rectification in I-V characteristics for weakly coupled spatially separated donor-acceptor systems [11]. Different coupling strengths of these sites to the electrodes result in the rectification effect in these molecular junctions. In this work, for the first time, we have carried out the study to find Coulomb blockade, NDC and rectification behaviour in the same system depending on the spatial coupling sites to the electrodes and also show that such I-V characteristics can be controlled and varied by external perturbations, like applying optical magnetic field and varying Gate voltage. Effectively, our work demonstrates these molecules as weakly coupled field effect transistors, where through external perturbation, its I-V characteristics can be controlled effectively to obtain a variety of interesting device characteristics.

Results and Discussion: Describe significant experimental and/or theoretical research advances or findings and their significance to the field and what work may be performed in the future as a follow on project. Fellow researchers will be interested to know what impact this research has on your particular field of science.

As discussed, we have used Kinetic equation approach to calculate the I-V characteristics. To reduce the computational efforts, we have used total number of electrons and their Sz value, as the quantum numbers. We diagonalize the Hamiltonian matrix in each of the N and Sz_tot sectors and consider two such appropriate sectors to calculate the current value. The bias is the source drain bias and we considered the effect of it on the molecular device by solving discrete Poisson equation self-consistently, but we find that I-V characteristics do not change at all with this. In fact, it is because the molecule is too small to sustain electrostatic interaction and so the molecular levels experience the average voltage, which is zero in our case. Effectively, the bias voltage affects the probability distribution of charge carriers through the Fermi-Dirac distribution function which is included in the rate equations. Interestingly, the charge carrier density get affected and so the Fermi-Dirac distribution function, if we add charge carriers through Gate electrode. We also have applied the optical magnetic field, through Peierls phase, which goes into the Hamiltonian with variation in kinetic energy term.

The Hamiltonian and relevant equations for Kinetic equation approach are given below.

The Hubbard Hamiltonian used for the study can be written as.

$$\mathbf{H} = \sum_{\mathbf{i=1}}^{\mathbf{2}} (\epsilon_{\mathbf{i}} - \mathbf{eW_g})\mathbf{a_i^\dagger a_i} + \sum_{\sigma=\uparrow,\downarrow} -\mathbf{t}(\mathbf{a_{1\sigma}^\dagger a_{2\sigma}} + \mathbf{h.c.}) + \mathbf{U}\sum_{\mathbf{i=1}}^{\mathbf{2}} \mathbf{n_{i\uparrow} n_{i\downarrow}}$$

where first term takes into account the orbital energy and Gate bias values, the second term is kinetic energy term in terms of hopping and the last term is the on-site Coulomb repulsion term, U. Each of the parameters for different atoms are considered in appropriate manner and has been verified with numbers from literature, thoroughly.

After solving the Hamiltonian and diagonalizing the Hamiltonian matrix, we obtain a set of eigenvalues

and eigenvectors. After this, we solve the rate equation by calculating the rate of transition of charges (either electron or hole) from the device to either of the electrodes. The corresponding equations are given below.

$$\Sigma^{L+}_{s'\rightarrow s} = \Gamma f_L(E_s - E'_s) \sum_{\sigma} | < s|C^{\dagger}_{1\sigma}|s' > |^2$$
$$\Sigma^{L-}_{s\rightarrow s'} = \Gamma(1 - f_L(E_s - E'_s)) \sum_{\sigma} | < s|C^{\dagger}_{1\sigma}|s' > |^2$$
$$\Sigma^{R+}_{s'\rightarrow s} = \Gamma f_R(E_s - E'_s) \sum | < s|C^{\dagger}_{N\sigma}|s' > |^2$$
$$\Sigma^{R-}_{s\rightarrow s'} = \Gamma(1 - f_R(E_s - E'_s)) \sum_{\sigma} | < s|C^{\dagger}_{N\sigma}|s' > |^2$$

where the notations are self-explanatory. L(R) correspond to the left (right) electrodes and + (-) correspond to electron (hole) going to the respective electrode. The Fermi-Dirac distribution function of the respective electrode at corresponding device energy values multiply with the probability of carrier transition to (from) the respective electrodes through the adjacent sites are explicitly calculated.

The total rate is then calculated summing all the transition rates

$$\Sigma_{s\rightarrow s'} = \Sigma^{L+}_{s\rightarrow s'} + \Sigma^{R+}_{s\rightarrow s'} + \Sigma^{L-}_{s\rightarrow s'} + \Sigma^{R-}_{s\rightarrow s'}$$

Then with a constraint that at the steady state when the measurement is made, the total probability of current to either of the electrodes is 1, at a time, one solves for the current equation as given below.

$$I_{\alpha} = e \sum_{s,s'} \Sigma^{\alpha+}_{s'\rightarrow s} P_{s'} - \Sigma^{\alpha-}_{s\rightarrow s'} P_s \qquad\qquad \alpha = L/R$$

This way, the current obtained in both the electrodes is same. We initiate the calculations for a device by fixing a value for the Gate bias, which in turn fixes the number of electrons in the device. The same set of calculations was carried again for another Gate bias. In fact, for a field effect transistor, the source-drain current is measured for a given Gate bias. We also do the same calculations for our device; calculate the current between weakly coupled source and drain electrodes at a given Gate bias value. This way the number of electrons in the device can be tuned to obtain I-V characteristics.

Figure 1. Schematic structures of naphthalenes and (BN) substituted naphthalenes.

We have successfully implemented this method and have calculated I-V characteristics for two sets of molecular systems as the device (6 and 10 member rings). Since this formalism is for the weak coupling regime, the electrode can be placed at any site of the device. Interestingly, we have considered all the possibilities and present results for only a few. Effectively, for six member ring, we have 4 contact possibilities, namely, left right contacts being, B-B, N-N, C-C and B-N. Our results clearly indicate that the I-V curves strongly depend on the atomic nature of the sites, which are connected to the electrodes. When two coupling sites are different chemical species, prominent rectification of current appears. Importantly, when both the coupling sites are B atoms, we find the appearance of NDC in the device. We discuss the results based on (i) charge densities at the coupling sites, (ii) transition rates among different many-body states, and (iii) the population probability of relevant many-body states. Further, we also demonstrate the modulation of current conduction by applying perpendicular magnetic field and gate voltage. Depending on the strength of magnetic field and gate voltage, we find a number of interesting features, arising in the I-V characteristics. In case of Napthalene molecular devices, we have considered 3 more analogues systems, namely, two pairs of (BN) substitutions at the center and at the terminal carbons and three pairs of (BN) substitutions (see Fig. 1). However, for Napthalene and its B-N analogues, we had to do some additional programming since the basis set for 10 member ring is quite large. We restricted our basis set to N, N+1 and N-1 number of electrons (where N is the number of electrons when the system is half-filled) and have considered 300 lowest energy values and their corresponding eigenstates in each subspace for the computation of current. We have verified with keeping all the states and find that the results are highly accurate.

Thus, in this work, we have successfully demonstrated various non-linear transport behaviour (Coulomb staircase, rectification and switching) appear for an intrinsically asymmetric heteronuclear cyclic field effect transistor molecular junction.

To summarize the results, in the case of Benzene analogues, we find:

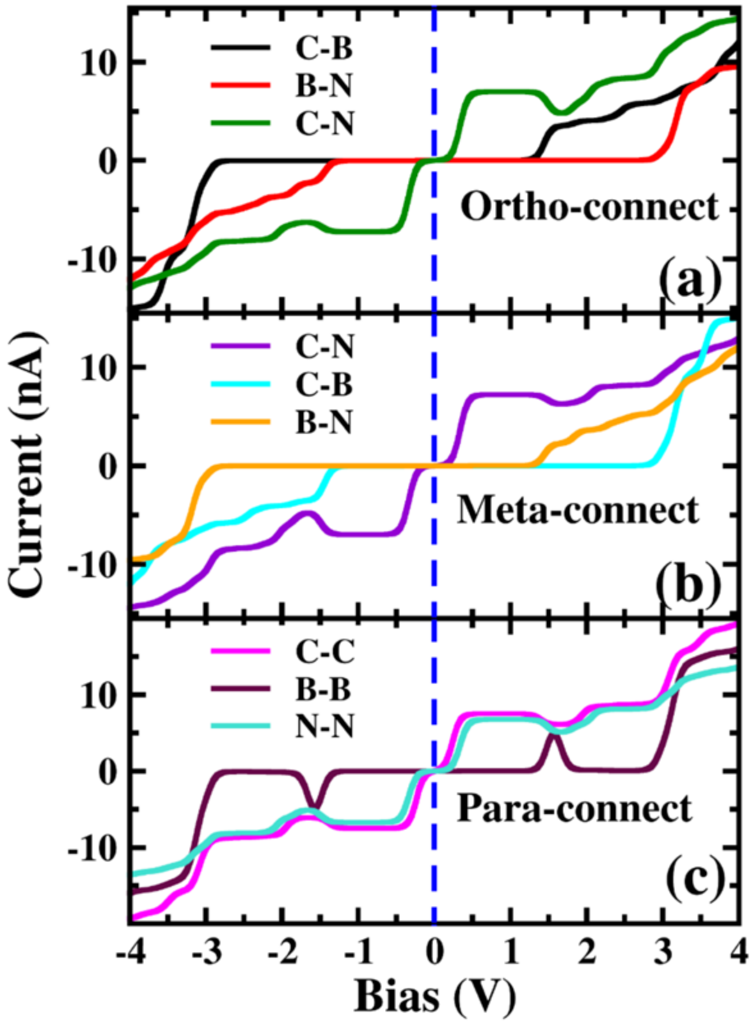


FIG. 2. Current (I) - source-drain voltage (V_{SD}) characteristics of molecular device where electrodes are connected in (a) ortho, (b) meta and (c)para-position. Blue dash lines represents the V_{SD} = 0.0. In the upper left insets of (a-c), the atomic sites where the electrodes are attached are shown.

(a) When para position Boron atoms are connected to electrodes, one finds symmetric negative differential conductance properties in I-V characteristics, which has been earlier seen in strongly coupled double quantum dots experimentally. Here this occurs due to the Boron sites which act as Lewis bases. When an optical magnetic field is applied, for small field, the current amplifies in the low bias window, but at a bias regime, where NDC was seen, the NDC peak weakens with increase in magnetic field strength and beyond a certain field strength, the NDC peak vanishes. Interestingly, without the magnetic field, the NDC peak can be switched on and switched off, by varying the Gate voltage.

(b) When the chemically asymmetric ortho positioned Boron and Nitrogen atoms are connected to electrodes on either side, one finds rectification in I-V characteristics. Even with switching on the magnetic field or Gate voltage, such rectification characteristics do not change.

(c) However, when two para positioned Carbon atoms are connected with the electrodes, one finds staircase behavior; i.e., one electron tunnels at a time and such behavior is quite characteristic of conjugated molecular systems.

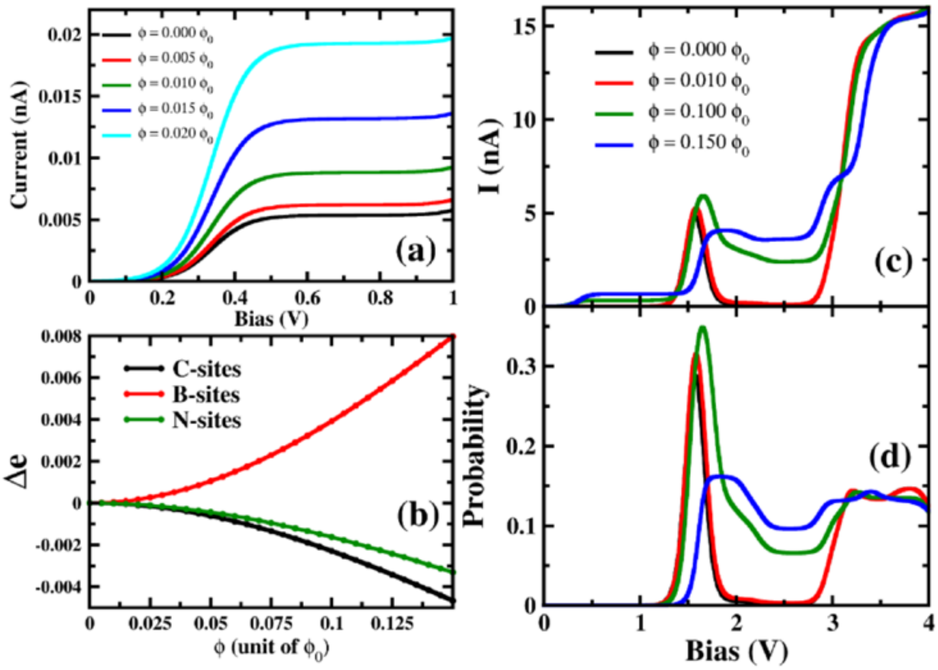


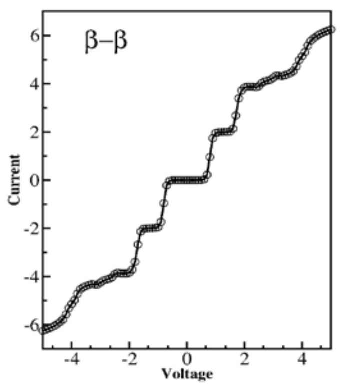
Fig. 3. (a) Current (I) under V_{SD} of $0V < V_{SD} < 1.0V$ with magnetic field of various strength for para positioned boron connected device. (b) Charge density at boron sites with varying magnetic field strength. (c) Current and (d) occupation probabilities of 7e-state under V_{SD} for magnetic field strength between 0.02 and 0.10.

(c) Application of a small magnetic field amplify the current in a low bias window (see Fig. 3a) and NDC behavior remains unaltered at low bias.

(d) With the increase in the magnetic field, nature of the current conduction changes in the region of NDC.

The salient results for Napthalene and its B-N analogues are the following:

We connect the lead to atoms on two different chains in naphthalene even though the results do not change with the same chain connectivity.



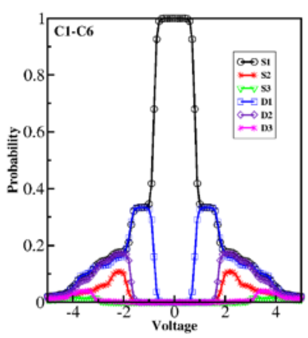


Fig. 4. I- V characteristics for C1-C6 connectivity.

(a) **Staircase like Coulomb blockade behaviors**: When the leads are connected to the terminal sites (β and β on opposite sides), with the application of bias, the probability of occupation for N electron ground state decreases drastically and that of N+1 electron state increases sharply indicating the single electron transfer from one electrode to the other and hence there is a peak in the I-V characteristics. It is followed by a plateau region whose width depends upon the energy gap between the first state and the second state in the (N+1) space. The next peak arises when the bias applied corresponds to the resonance energy of the higher excited state.

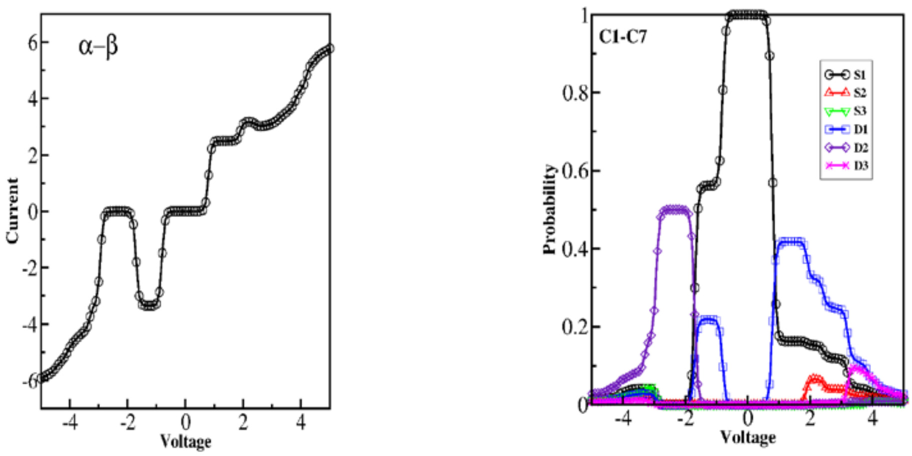


Fig. 5 . I- V characteristics for C1-C7 connectivity.

(b) **Rectification**: When the leads are connected to α and β sites of the 10 member ring, there is a slight increase in the current initially and with further increase in bias, the current decreases suddenly and then increases. This is the case either for positive bias or for negative bias. However, at higher bias, the I-V nature is the same as like staircase behavior. The increase and decrease in current for either positive or negative bias appears because, the probability of occupation of excited state in the doublet space increases at the resonant transition, whereas the probability of the ground N electron state and N+1 electron state decrease drastically.

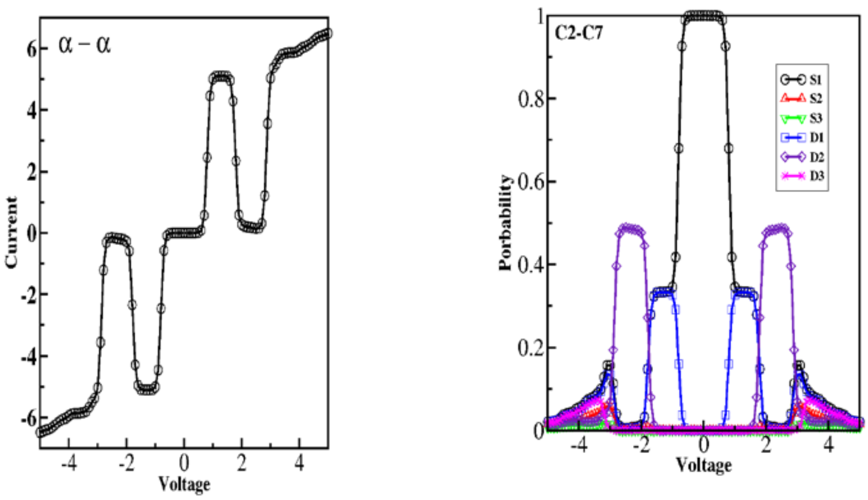


Fig. 6 . I- V characteristics for C2-C7 connectivity.

(c) Negative differential conductivity: When the leads are connected to α and α sites, the NDC appears for both positive and negative bias values. If the leads are connected to different atoms, they are quite asymmetric. Here again such behavior arises as the probability of occupation of excited state of doublet space increases and those of ground state singlet and the doublet space decreases at those positive and nagative bias values.

(d) In all the cases, if the leads are connected to different atoms (among Carbon, Boron and Nitrogen), the peak values are asymmetric with respect to both the magnitude of the bias and the intensity of the current (both magnitude in x and y axes).

List of Publications and Significant Collaborations that resulted from your AOARD supported project: In standard format showing authors, title, journal, issue, pages, and date, for each category list the following:
a) papers published in peer-reviewed journals,
b) papers published in non-peer-reviewed journals or in conference proceedings,
c) conference presentations,
d) manuscripts submitted but not yet published, and
e) provide a list any interactions with industry or with Air Force Research Laboratory scientists or significant collaborations that resulted from this work.

We have worked on two projects to design nanoscale field effect transistors by considering effectively two organic molecular systems and substituting donor, acceptor atoms and generating a number of their analogues, keeping the whole system iso electronic. In fact, these donor and acceptor atoms transfer charges and thereby make these systems perfect charge transfer molecular system which would be ideal for application purposes. In fact, we have found a number of exotic field effect transistor I-V characteristics, which are quite interesting from applications point of view. Field effect transistor is defined as a device where current or conductance can be controlled by external input, i.e., Gate voltage. We have obtained I-V characteristics, namely, staircase, NDC, rectification behaviors, which signifies a transistor which can act as nanoscale memory device or switching device, apart from its classical transistor characteristics.

We have two manuscripts written on these, where we have acknowledged AOARD for financial assistance. In fact, one of them have been submitted and the other will be submitted soon. The details of the two manuscripts are

(1) D. Ghosh. P. Parida and Swapan K Pati, "Small Heterocyclic Molecule as Multistate Transistor: A Quantum Many Body Approach", Submitted (2016)

(2) Y. Anusooya Pati and Swapan K Pati, "From Molecular electronics to Field Effect Transistor: Case Studies for Napthalene and its B-N analogues".

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